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J. Frederic Bonnans, Xiaolu Tan. Monotonicity condition for the  $\theta$ -scheme for diffusion equations. [Research Report] RR-7778, INRIA. 2011, pp.6. [inria-00634417](https://hal.inria.fr/inria-00634417)

**HAL Id: [inria-00634417](https://hal.inria.fr/inria-00634417)**

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Submitted on 21 Oct 2011

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***Monotonicity condition for the  $\theta$ -scheme  
for diffusion equations***

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**N° 7778**

Octobre 2011

Thème NUM

 ***rapport  
de recherche***



## Monotonicity condition for the $\theta$ -scheme for diffusion equations\*

J. Frédéric BONNANS<sup>†</sup>, Xiaolu TAN<sup>‡</sup>

Thème NUM — Systèmes numériques  
Équipes-Projets Commands

Rapport de recherche n° 7778 — Octobre 2011 — 6 pages

**Abstract:** We derive the necessary and sufficient condition for the  $L^\infty$ –monotonicity of finite difference  $\theta$ -scheme for a diffusion equation. We confirm that the discretization ratio  $\Delta t = O(\Delta x^2)$  is necessary for the monotonicity except for the implicit scheme. In case of the heat equation, we get an explicit formula, which is weaker than the classical CFL condition.

**Key-words:** Theta-scheme, monotonicity.

\* We thank Nizar Touzi (CMAP) for fruitful discussions.

<sup>†</sup> INRIA-Saclay and CMAP, École Polytechnique, 91128 Palaiseau, and Laboratoire de Finance des Marchés d'Énergie, France (Frederic.Bonnans@inria.fr).

<sup>‡</sup> CMAP, École Polytechnique, 91128 Palaiseau, France (xiaolu.tan@polytechnique.edu), research supported by the Chair *Financial Risks* of the *Risk Foundation* sponsored by Société Générale, the Chair *Derivatives of the Future* sponsored by the Fédération Bancaire Française, and the Chair *Finance and Sustainable Development* sponsored by EDF and CA-CIB.

## La condition de la monotonie du $\theta$ –schéma pour les équations de diffusion

**Résumé :** Nous nous intéressons à la condition nécessaire et suffisante de la monotonie du  $\theta$ –schéma pour l'équation de diffusion en dimension un. Notre résultat confirme que le ratio de discrétisation  $\Delta t = O(\Delta x^2)$  est nécessaire pour la monotonie sauf le schéma implicite. Dans le cas de l'équation de la chaleur, nous obtenons la formule explicite, qui est plus faible que la condition CFL.

**Mots-clés :** Theta-schéma, monotonie.

## 1 Introduction

The monotonicity of a numerical scheme is an important issue in numerical analysis. For example, in the convergence analysis in Chapter 2 of Allaire [1], the author uses the  $L^\infty$ –monotonicity to derive the stability of the scheme, which gives a proof of convergence. In the viscosity solution convergence context of Barles and Souganidis [2], the  $L^\infty$ –monotonicity is a key criterion to guarantee the convergence of the numerical scheme.

We are here interested in the finite difference  $\theta$ –scheme for the diffusion equation:

$$\partial_t v - \sigma^2(x) D_{xx}^2 v = 0, \quad (t, x) \in \mathbb{R}^+ \times \mathbb{R}. \quad (1.1)$$

with initial condition  $v(0, x) = g(x)$ .

## 2 The $\theta$ –scheme and CFL condition

Let  $h = (\Delta t, \Delta x) \in (\mathbb{R}^+)^2$  be the discretization in time and space, denote  $t_n := n\Delta t$ ,  $x_i := i\Delta x$ ,  $\sigma_i := \sigma(x_i)$  and by  $u_i^n$  the numerical solution of  $v$  at point  $(t_n, x_i)$ , let  $\mathcal{N} := \{x_i : i \in \mathbb{N}\}$  be a discrete grid on  $\mathbb{R}$ . The finite difference  $\theta$ –scheme ( $0 \leq \theta \leq 1$ ) for diffusion equation (1.1) is a countable infinite dimensional linear system on  $\mathcal{N}$ :

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} - \sigma_i^2 \left( \theta \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} + (1 - \theta) \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \right) = 0, \quad (2.1)$$

with initial condition  $u_i^0 = g(x_i)$ .

Let  $(u^n) := (u_i^n)_{i \in \mathbb{Z}}$  be a  $\mathbb{Z}$ –dimensional vector, denote  $\alpha_i := \frac{\sigma_i^2 \Delta t}{\Delta x^2}$  and  $\beta_i := \frac{\theta \alpha_i}{1 + 2\theta \alpha_i}$ , we define  $\mathbb{Z} \times \mathbb{Z}$  diensional matrices  $I$ ,  $D$ ,  $T$  and  $E$  as follows:  $I$  is the identity matrix,  $D$  is a diagonal matrix with  $D_{i,i} = \alpha_i$ ,  $T$  is a tridiagonal matrix with  $T_{i,i-1} = T_{i,i+1} = \alpha_i$  and  $T_{i,i} = 0$ , and  $E := \theta[I + 2\theta D]^{-1}T$  which is a tridiagonal matrix with  $E_{i,i-1} = E_{i,i+1} = \beta_i$  and  $E_{i,i} = 0$ . Then the system (2.1) can be written as

$$[I + 2\theta D - \theta T] (u^{n+1}) = [I - 2(1 - \theta)D + (1 - \theta)T] (u^n),$$

or equivalently

$$[I + 2\theta D] [I - E] (u^{n+1}) = [I - 2(1 - \theta)D + (1 - \theta)T] (u^n). \quad (2.2)$$

**Proposition 2.1.** *Suppose that the function  $g$  is bounded on  $\mathcal{N}$  and there is constant  $\bar{\sigma} > 0$  such that  $|\sigma_i| \leq \bar{\sigma}$  for every  $i \in \mathbb{Z}$ , then the  $\mathbb{Z} \times \mathbb{Z}$  matrix  $I - E$  is invertible and its inversion  $B$  is given by*

$$B := I + \sum_{n=1}^{\infty} E^n. \quad (2.3)$$

And therefore, there is a unique solution for system (2.1) (or (2.2)) given by

$$(u^{n+1}) = B [I + 2\theta D]^{-1} [I - 2(1 - \theta)D + (1 - \theta)T] (u^n). \quad (2.4)$$

**Proof.** First,  $(\alpha_i)_{i \in \mathbb{N}}$  defined by  $\alpha_i = \frac{\sigma_i^2 \Delta t}{\Delta x^2}$  are uniformly bounded by  $\bar{\alpha} := \frac{\bar{\sigma}^2 \Delta t}{\Delta x^2}$  since  $(\sigma_i)_{i \in \mathbb{Z}}$  are uniformly bounded by  $\bar{\sigma}$ . It follows that  $\beta_i = \frac{\theta \alpha_i}{1 + 2\theta \alpha_i} \leq \rho := \frac{\theta \bar{\alpha}}{1 + 2\theta \bar{\alpha}} < \frac{1}{2}$ .

Denote by  $B(\mathcal{N})$  the space of all bounded functions defined on  $\mathcal{N}$ , then  $E$  can be viewed as an operator on  $B(\mathcal{N})$  and its  $L^\infty$ -norm is defined by

$$\|E\|_\infty := \sup_{u \in B(\mathcal{N}), u \neq 0} \frac{|Eu|_\infty}{|u|_\infty}.$$

Clearly,  $\|E\|_\infty \leq 2\rho < 1$ , and therefore,  $B$  in (2.3) is well defined and one can easily verify that  $B$  is the inverse of  $[I - E]$ .  $\square$

**Definition 2.2.** A numerical scheme for equation (1.1) given by  $u_i^{n+1} = \mathbf{T}_h[u^n]_i$  is said to be  $L^\infty$ -monotone if

$$u_i^{1,n} \leq u_i^{2,n}, \quad \forall i \in \mathbb{Z} \quad \Rightarrow \quad \mathbf{T}_h[u^{1,n}]_i \leq \mathbf{T}_h[u^{2,n}]_i, \quad \forall i \in \mathbb{Z}.$$

**Remark 2.3.** It is well-known that in the case  $\theta = 1$ , system (2.2) is an implicit scheme, and it is automatically  $L^\infty$ -monotone for every discretization  $(\Delta t, \Delta x)$ . When  $\theta < 1$ , a sufficient condition to guarantee the  $L^\infty$ -monotonicity of system (2.2) is the CFL (Courant-Friedrichs-Lewy) condition

$$\bar{\alpha} := \frac{\bar{\sigma}^2 \Delta t}{\Delta x^2} \leq \frac{1}{2(1-\theta)}, \quad \text{for } \bar{\sigma} := \sup_{i \in \mathbb{Z}} \sigma_i. \quad (2.5)$$

The CFL condition is a sufficient condition for the monotonicity of  $\theta$ -scheme, and it implies a discretization ratio  $\Delta t = O(\Delta x^2)$ . We shall confirm that this ratio is necessary to guarantee the monotonicity in the following.

### 3 The necessary and sufficient condition

Let  $\gamma_i := \frac{(1-\theta)\alpha_i}{1+2\theta\alpha_i} = \frac{(1-\theta)}{\theta}\beta_i$  and  $b_{i,j}$  be elements of the matrix  $B$ , i.e.  $B = (b_{i,j})_{(i,j) \in \mathbb{Z}^2}$ . It is clear that  $b_{i,j} \geq 0$  for every  $(i,j) \in \mathbb{Z}^2$  by the definition of  $B$  in (2.3). Therefore, it follows from (2.4) that the necessary and sufficient condition for monotonicity of system (2.1) can be written as :

$$b_{i,j-1}\gamma_{j-1} + b_{i,j}\left(\frac{1}{1+2\theta\alpha_j} - 2\gamma_j\right) + b_{i,j+1}\gamma_{j+1} \geq 0, \quad \forall (i,j) \in \mathbb{Z}^2. \quad (3.1)$$

**Theorem 3.1.** Suppose that  $|\sigma_i| \leq \bar{\sigma} < \infty$  for every  $i \in \mathbb{Z}$ , and let  $\theta \in (0,1)$ . Then the necessary and sufficient condition of monotonicity for the  $\theta$ -scheme in (2.1) is

$$\alpha_i = \frac{\sigma_i^2 \Delta t}{\Delta x^2} \leq \frac{1}{2(1-\theta)} + \frac{b_{i,i} - 1}{2\theta(1-\theta)}, \quad \forall i \in \mathbb{Z}. \quad (3.2)$$

**Proof.** First, since  $B$  is the inversion of  $I - E$ , we have  $B[I - E] = I$ , and it follows that

$$b_{i,j-1}\beta_{j-1} + b_{i,j+1}\beta_{j+1} = \begin{cases} b_{ij} - 1, & \text{for } i = j, \\ b_{ij}, & \text{for } i \neq j. \end{cases}$$

Therefore, in case that  $i \neq j$ , (3.1) is equivalent to:

$$b_{i,j} \left( \frac{1-\theta}{\theta} + \frac{1}{1+2\theta\alpha_j} - 2\gamma_j \right) \geq 0. \quad (3.3)$$

Since  $b_{i,j} \geq 0$ , the inequality (3.3) holds as soon as

$$(1 - \theta)(1 + 2\theta\alpha_j) + \theta - 2\theta(1 - \theta)\alpha_j \geq 0,$$

which is always true.

In case that  $i = j$ , (3.1) is equivalent to:

$$b_{i,i} \left( \frac{1 - \theta}{\theta} + \frac{1}{1 + 2\theta\alpha_i} - 2\gamma_i \right) - \frac{1 - \theta}{\theta} \geq 0,$$

i.e.

$$\alpha_i \leq \frac{1}{2(1 - \theta)} + \frac{b_{i,i} - 1}{2\theta(1 - \theta)}.$$

which is the required inequality (3.2).  $\square$

**Remark 3.2.** Since  $b_{i,i} < \infty$  for every  $i \in \mathbb{Z}$ , it follows from Theorem 3.1 that the ratio  $\Delta t = O(\Delta x^2)$  is necessary for the monotonicity of  $\theta$ -scheme ( $0 < \theta < 1$ ) as soon as  $\sigma_i \neq 0$  for some  $i \in \mathbb{Z}$ .

## 4 The heat equation

In this section, let us suppose that  $\sigma(x) \equiv \sigma_0$  with a positive constant  $\sigma_0$ , then the diffusion equation turns to be the heat equation:

$$\partial_t v - \sigma_0^2 D_{xx}^2 v = 0, \quad (t, x) \in \mathbb{R}^+ \times \mathbb{R}. \quad (4.1)$$

In this case, we can compute  $b_{i,i}$  and then get an explicit formula for the monotonicity condition (3.2). Let

$$A \text{ be a } \mathbb{Z} \times \mathbb{Z} \text{ tridiagonal matrix such that } A_{i,i-1} = A_{i,i+1} = 1 \text{ and } A_{i,i} = 0, \quad (4.2)$$

then clearly,  $E = \beta A$  with  $\beta = \frac{\theta\alpha}{1+2\theta\alpha} < \frac{1}{2}$ ,  $\alpha = \frac{\sigma_0^2 \Delta t}{\Delta x^2}$  and

$$B = [I - \beta A]^{-1} := \sum_{n=0}^{\infty} \beta^n A^n. \quad (4.3)$$

**Lemma 4.1.** Denote by  $A^n$  the  $n$ -th exponentiation of matrix  $A$  in (4.2) for  $n \in \mathbb{N}$ , we rewritten  $A^n = (a_{i,j}^{(n)})_{(i,j) \in \mathbb{Z} \times \mathbb{Z}}$ . Then,

$$a_{i,j}^{(n)} = \begin{cases} C_n^{(n+i-j)/2}, & \text{if } \frac{n+i-j}{2} \in \mathbb{Z} \cap [0, n], \\ 0, & \text{otherwise.} \end{cases} \quad (4.4)$$

**Proof.** We proceed by induction. First, it is clearly that (4.4) holds true for  $n = 1$ . Suppose that the (4.4) is true in case that  $n = m$ . Since  $A^{m+1} = A^m A$ , we then have  $a_{i,j}^{m+1} = a_{i,j-1}^m + a_{i,j+1}^m$ . It follows from  $C_n^k = C_{n-1}^k + C_{n-1}^{k-1}$  that (4.4) holds still true for the case  $n = m + 1$ . We then conclude the proof.  $\square$

By Lemma 4.1 and equality (4.3), we get  $b_{i,i} = \sum_{k=0}^{\infty} C_{2k}^k \beta^{2k}$  with the convention that  $C_0^0 := 1$ . As a result, the monotonicity condition (3.2) of  $\theta$ -scheme reduces to

$$\alpha \leq \frac{1}{2(1 - \theta)} + \frac{f(\beta)}{2\theta(1 - \theta)}, \quad (4.5)$$



where

$$f(x) := \sum_{k=1}^{\infty} C_{2k}^k x^{2k} \quad \text{for } -\frac{1}{2} < x < \frac{1}{2}.$$

**Remark 4.2.** We can verify that  $C_{2k}^k \approx \frac{1}{\sqrt{\pi k}} 4^k$  as  $k \rightarrow \infty$  by Stirling's formula, thus the radius of convergence of  $f(x)$  is  $\frac{1}{2}$ .

Let us now compute the function  $f(x)$ . Since  $C_{2k}^k = 2^{\frac{2k-1}{k}} C_{2(k-1)}^{k-1}$ , it follows that for  $|x| < \frac{1}{2}$ ,

$$\begin{aligned} f'(x) &= \sum_{k=1}^{\infty} 2k C_{2k}^k x^{2k-1} = \sum_{k=1}^{\infty} 4(2k-1) C_{2(k-1)}^{k-1} x^{2k-1} \\ &= 4x + \sum_{k=1}^{\infty} (8k+4) C_{2k}^k x^{2k+1} = 4x + 4x^2 f'(x) + 4x f(x). \end{aligned}$$

We are then reduced to the ordinary differential equation

$$f'(x) = \frac{4x}{1-4x^2} (f(x) + 1), \quad \text{with } f(0) = 0,$$

whose solution is  $f(x) = \frac{1}{\sqrt{1-4x^2}} - 1$ . Inserting this solution into (4.5), and by a direct manipulation, it follows that (4.5) is equivalent to

$$\alpha \leq \frac{1}{2(1-\theta)} + \frac{\theta}{4(1-\theta)^2}. \quad (4.6)$$

We get the following theorem:

**Theorem 4.3.** The necessary and sufficient condition for the  $L^\infty$ -monotonicity of  $\theta$ -scheme ( $0 < \theta < 1$ ) of the heat equation (4.1) is

$$\alpha = \frac{\sigma_0^2 \Delta t}{\Delta x^2} \leq \frac{1}{2(1-\theta)} + \frac{\theta}{4(1-\theta)^2}. \quad (4.7)$$

**Remark 4.4.** In particular, when  $\theta = \frac{1}{2}$ , the CFL condition is  $\alpha = \frac{\sigma_0^2 \Delta t}{\Delta x^2} \leq 1$ , and the necessary and sufficient condition of the monotonicity is  $\alpha = \frac{\sigma_0^2 \Delta t}{\Delta x^2} \leq \frac{3}{2}$ .

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Centre de recherche INRIA Saclay – Île-de-France  
Parc Orsay Université - ZAC des Vignes  
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Éditeur  
INRIA - Domaine de Voluceau - Rocquencourt, BP 105 - 78153 Le Chesnay Cedex (France)  
<http://www.inria.fr>  
ISSN 0249-6399